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Non-Markovian quantum dissipation in the Kraus representation

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Abstract. – In order to describe the evolution of a quantum system that is coupled to a reservoir, a non-phenomenological Kraus map is constructed. At time zero, system and reservoir are not entangled. In the perturbative series for the density operator of the system all reservoir correlation functions are factorised into products of pair-correlation functions. This allows for a resummation of the perturbative series up to infinite order. The density operator can be expressed in terms of an auxiliary system operator that satisfies an analytically tractable integral equation. Hence, the difficulties caused by integral kernels of Nakajima-Zwanzig type are circumvented. Assuming an interaction between system and reservoir of the Jaynes-Cummings form, one shows that the Kraus map is capable of generating Rabi oscillations of a two-level atom. If the reservoir is a continuum, the Kraus map reproduces the Wigner-Weisskopf theory of spontaneous emission.

Introduction. – More than 30 years ago, Kraus [1] made an important contribution to the field of nonrelativistic quantum dissipation. He recognised that the evolution in time t of the density operator $\rho_S(t)$ of an open quantum system S is governed by the map

$$\rho_S(t) = \sum_m W_m(t) \rho_S W_m^\dagger(t). \quad (1)$$

This representation embodies the principle of complete positivity [2], which is now receiving full attention, in particular from the community working on quantum computing and quantum decoherence [3–5]. For a system that is initially entangled with its surroundings, the validity of (1) was questioned [6, 7].

The relation between the set of evolution operators $\{W_m(t)\}$ and the unitary dynamics of ordinary quantum mechanics can be established in a standard manner [8]. The system S is coupled to a reservoir R such that the composite SR of system and reservoir is in the factorised state $\rho_S \otimes \rho_R$ at time zero. Subsequently, one lets the composite evolve with the Heisenberg equation. As the evolution of the reservoir is of no concern to the experimentalist, the partial trace over R is taken. Upon moving to the interaction picture, one obtains

$$\rho_S(t) = \text{Tr}_R [e^{iH_0 t} e^{-iH t} \rho_S \otimes \rho_R e^{iH t} e^{-iH_0 t}]. \quad (2)$$

The Hamiltonian can be decomposed as $H = H_0 + \lambda H_1$. The constituents are given by

$$H_0 = H_S \otimes 1_R + 1_S \otimes H_R, \quad H_1 = \sum_{\alpha} V_{\alpha} \otimes U_{\alpha}. \quad (3)$$

The coupling constant λ is real. In order to meet the constraint $H_1^{\dagger} = H_1$, the system potentials $\{V_{\alpha}\}$ and the reservoir potentials $\{U_{\alpha}\}$ need not be self-adjoint.

To cast (2) into the form (1), one represents the initial state of the reservoir as $\rho_R = \sum_k \mu_k |r_k\rangle\langle r_k|$, where the eigenvalues $\{\mu_k\}$ are non-negative and add up to unity. As they make up an orthonormal basis for the Hilbert space of the reservoir, the vectors $\{|r_k\rangle\}$ can be employed for evaluation of the trace over R. For any two system vectors $|\phi\rangle$ and $|\chi\rangle$ one then finds

$$\langle\phi|W_{kl}(t)|\chi\rangle = \mu_l^{1/2} \langle\phi \otimes r_k|e^{iH_0 t} e^{-iH t}|\chi \otimes r_l\rangle. \quad (4)$$

The multi-index m appearing in (1) is made up by the integers k and l .

Usually, diagonalisation of H is not feasible, so that an exact computation of (2) can only happen numerically. If one wants to avoid that, concessions must be made. The oldest remedy is the van Hove [9] limit $t \rightarrow \infty$ and $\lambda \rightarrow 0$, with the scaled time $\lambda^2 t$ constant. From (2) one derives for t non-negative [10]

$$\lim_{\lambda \rightarrow 0} \rho_S(t/\lambda^2) = e^{(L_1 + L_2)t} \rho_S. \quad (5)$$

This is a semigroup that generates Markovian dynamics. The reservoir talks to the system through the pair-correlation function

$$c_{\alpha\beta}(t, s) = \text{Tr}_R [U_{\alpha}(t) U_{\beta}(s) \rho_R], \quad (6)$$

where the time-dependent potentials $U_{\alpha}(t) = \exp[iH_R t] U_{\alpha} \exp[-iH_R t]$ have been introduced. The generator L_1 depends on the Laplace transform of (6), whereas L_2 depends on the Fourier transform. Full expressions can be found in any textbook on this subject [8, 11]. By construction, the semigroup (5) complies with the Kraus map (1).

Construction of a Kraus map. – A serious drawback of taking the van Hove limit is the complete removal of any (quasi-)reversible behaviour. We are going to construct a Kraus map that allows for periodic energy exchange between system and reservoir as long as t is comparable to a typical decorrelation time of the reservoir. To gain such non-Markovian dynamics from (2), we eliminate the unitary operator on either side of $\rho_S \otimes \rho_R$ with the help of the perturbative expansion

$$\begin{aligned} e^{iH_0 t} e^{-iH t} &= \sum_{n=0}^{\infty} \sum_{\alpha_1 \alpha_2 \dots \alpha_n} (-i\lambda)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \dots \int_0^{t_{n-1}} dt_n \times \\ &\times V_{\alpha_1}(t_1) V_{\alpha_2}(t_2) \dots V_{\alpha_n}(t_n) \otimes U_{\alpha_1}(t_1) U_{\alpha_2}(t_2) \dots U_{\alpha_n}(t_n), \end{aligned} \quad (7)$$

where the notation $V_{\alpha}(t) = \exp[iH_S t] V_{\alpha} \exp[-iH_S t]$ has been employed. There is a simple reason for making use of (7) instead of the more common commutator-based expansion given on p. 79 of [11]. Any presence of repeated commutators spoils our chances of coming up with a realisation of (1).

After insertion of (7), reservoir correlation functions of arbitrarily high order appear in (2). We cannot afford to drop any of these, because it is the strong-coupling regime that we are interested in. On the other hand, we can afford to perform a factorisation into products

of pair-correlation functions (6). If all contractions of the Wick theorem [11] are retained, the structure of (2) remains complicated. We therefore propose to retain nearest-neighbour contractions only. In our perturbative expansion we systematically carry out the replacements

$$\begin{aligned} U_\alpha(t)U_\beta(s)\rho_R &\longrightarrow c_{\alpha\beta}(t,s)\rho_R, \\ \rho_R U_\beta^\dagger(s)U_\alpha^\dagger(t) &\longrightarrow c_{\alpha\beta}^*(t,s)\rho_R. \end{aligned} \quad (8)$$

During the process of factorising correlation functions, one should refrain from using the cyclic property of the trace over R. Then (1) is never endangered.

A correlation function containing $2p$ reservoir potentials on the left-hand side of ρ_R and $2q$ reservoir potentials on the right-hand side of ρ_R factorises into a product of p functions $c_{\alpha\beta}(t,s)$ and q functions $c_{\alpha\beta}^*(t,s)$. The integers p and q take on any value between zero and infinity. The corresponding terms of the perturbative expansion can be summed up to yield the product $Q(t,0)\rho_S Q^\dagger(t,0)$. The system operator $Q(t,0)$ is a perturbative series, which can be generated through iteration of the integral equation

$$Q(t, t_0) = 1_S - \lambda^2 \sum_{\alpha\beta} \int_{t_0}^t ds \int_{t_0}^s du V_\alpha(s) V_\beta(u) Q(u, t_0) c_{\alpha\beta}(s, u). \quad (9)$$

The time t_0 equals zero for the moment. The above equation can be solved within the Hilbert space of the system. Use is made of Laplace transformation. To that end, one writes the integral on the right-hand side of (9) as a convolution. One expands the potentials $\{V_\alpha\}$ in terms of the eigenstates of H_S , and performs the shift $c_{\alpha\beta}(s, u) = c_{\alpha\beta}(s - u, 0)$. The last relation is a consequence of the standard [11] assumption that ρ_R and H_R commute.

Next, we turn to correlation functions containing an odd number of reservoir potentials on one side or either side of ρ_R . For the first category employment of (8) gives a vanishing result. This is caused by the circumstance that quite often the one-potential average $\text{Tr}_R[U_\alpha(t)\rho_R]$ equals zero. If it does not, one should invoke the assumption $[\rho_R, H_R] = 0$, and transfer the operator $\text{Tr}_R(H_1\rho_R)$ to the system Hamiltonian.

For the second category systematic use of (8) leads to a remaining factor of the form $\text{Tr}_R[U_\alpha(s)\rho_R U_\beta^\dagger(u)]$. It can be rendered identical to (6) by utilising the self-adjointness of H_1 as well as the cyclic property of the trace. Now we are in a position to sum up all terms of our perturbative expansion for the density operator (2). The outcome reads

$$\rho_S(t) = Q(t,0)\rho_S Q^\dagger(t,0) + \lambda^2 \sum_{\alpha\beta} \int_0^t ds \int_0^t du V_\alpha(s) Q(s,0) \rho_S Q^\dagger(u,0) V_\beta(u) c_{\beta\alpha}(u, s). \quad (10)$$

One verifies that upon substituting the iterative solution of (9) into (10), all terms of (2) emerge. Hence, in evaluating the density operator (2), we made one concession only. Instead of taking the van Hove limit, we carried out the replacements (8). As evidenced by (2), we assumed that system and reservoir are not entangled at time zero.

We emphasise that (9) and (10) depend on the reservoir operators through the presence of pair-correlation functions. By construction, (10) is a Kraus map, so surely the density operator is self-adjoint and positive. The identity $d \text{Tr}_S \rho_S(t)/dt = 0$, which is a direct consequence of (9) and (10), guarantees that the trace is conserved. Hence, for any Hamiltonian the map (10) generates physically meaningful dynamics. To demonstrate its non-Markovian character, we work out a specific example.

Dissipative dynamics of a two-level atom. – For S we choose a two-level atom with $H_S = \omega_A(i_+ - i_-)/2$ and for R an electromagnetic mode with $H_R = \omega_F a^\dagger a$. We assume the Jaynes-Cummings interaction [12]

$$H_1 = \sigma_+ \otimes a + \sigma_- \otimes a^\dagger. \quad (11)$$

The four matrices

$$i_+ = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad i_- = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad (12)$$

generate all atomic operators. The ladder operators a, a^\dagger satisfy the boson commutation relation $[a, a^\dagger] = 1$. The difference between the atomic frequency ω_A and the field frequency ω_F is measured by the detuning parameter $\Delta = (\omega_A - \omega_F)/(2\lambda)$. We let the field start from the photon-number state $\rho_R = |p\rangle\langle p|$, with p any non-negative integer. One checks that two pair-correlation functions differ from zero, namely $c_{12}(t, s) = (p+1)\exp[-i\omega_F(t-s)]$ and $c_{21}(t, s) = p\exp[i\omega_F(t-s)]$.

Swift solution of (9) can happen by means of Laplace transformation. Introducing the abbreviations $d_p(t) = c_p(t) - i\Delta s_p(t)$, $c_p(t) = \cos(w_p t)$, $s_p(t) = \sin(w_p t)/w_p$, and $w_p = (p + \Delta^2)^{1/2}$, one can express the solution of (9) as

$$Q(t, 0) = e^{i\Delta\lambda t} d_{p+1}(\lambda t) i_+ + e^{-i\Delta\lambda t} d_p^*(\lambda t) i_- . \quad (13)$$

By evaluating (10), one fixes the density operator. Its independent components are given by

$$\begin{aligned} i_+ \rho_S(t) i_+ &= |d_{p+1}(\lambda t)|^2 i_+ \rho_S i_+ + p s_p^2(\lambda t) \sigma_+ \rho_S \sigma_- , \\ i_+ \rho_S(t) i_- &= e^{2i\Delta\lambda t} d_p(\lambda t) d_{p+1}(\lambda t) i_+ \rho_S i_- . \end{aligned} \quad (14)$$

Precisely the same solutions are obtained from a direct diagonalisation of H [13]. They describe Rabi oscillations of the atom. Hence, we witness periodic energy exchange between system and reservoir, one of the hallmarks of non-Markovian behaviour. In case a coherent state is chosen for ρ_R , the outcome of the Kraus map deviates from the exact dynamics. Evaluation of $i_+ \rho_S(t) i_+$ with the help of (10) brings us once more to (14), with p equal to the squared norm of the coherence parameter. However, the exact atomic density operator exhibits the well-known collapses and revivals of the Rabi oscillations.

The foregoing positive conclusion incites us to find out whether the map (10) is also capable of generating purely Markovian dynamics. To show that the answer is affirmative, we couple a two-level atom to a continuum of modes. We replace (11) by

$$H_1 = \sigma_+ \otimes \int_0^\infty d\omega g(\omega) a(\omega) + \sigma_- \otimes \int_0^\infty d\omega g^*(\omega) a^\dagger(\omega). \quad (15)$$

The coupling strength $g(\omega)$ may be any smooth function falling off to zero for $\omega \rightarrow \infty$. The reservoir Hamiltonian is now $H_R = \int_0^\infty d\omega \omega a^\dagger(\omega) a(\omega)$, with commutators $[a(\omega), a(\omega')] = 0$ and $[a(\omega), a^\dagger(\omega')] = \delta(\omega - \omega')$. If the reservoir is kept at zero temperature, its initial state can be taken as $\rho_R = |0\rangle\langle 0|$. For t strictly positive, Laplace transformation of (9) yields $Q(t, 0) = i_- + f(t) i_+$ and

$$f(t) = \frac{i}{2\pi} \int_{-\infty}^\infty d\omega e^{-i\omega t} \left[\omega - \lambda^2 \int_0^\infty d\omega' \frac{|g(\omega')|^2}{\omega + \omega_A - \omega' + i\epsilon} \right]^{-1}. \quad (16)$$

As ϵ is infinitesimally positive, the integrand has a cut just below the real axis of the complex ω plane. This is a genuine sign of irreversibility. Indeed, by means of a Riemann-Lebesgue argument one proves that $f(t)$ converges to zero for large times.

With the help of (10) the density operator is determined as

$$i_+ \rho_S(t) i_+ = |f(t)|^2 i_+ \rho_S i_+, \quad i_+ \rho_S(t) i_- = f(t) i_+ \rho_S i_- . \quad (17)$$

The same expressions are obtained by performing a diagonalisation of H at zero temperature [11]. For large times, the atom decays to its ground state i_- . If one is not interested in the strong-coupling regime, one may take the van Hove limit. From (16) one derives $\lim_{\lambda \rightarrow 0} f(t/\lambda^2) = \exp[i\Omega t - \pi\Gamma t]$. The energy shift Ω and lifetime Γ^{-1} are given by the famous expressions $\mathcal{P} \int_0^\infty d\omega |g(\omega)|^2 / (\omega - \omega_A)$ and $|g(\omega_A)|^{-2}$, respectively. We see that the Kraus map (10) reproduces not only Rabi oscillations, but also the complete Wigner-Weisskopf theory of spontaneous emission.

Closing remarks. – i) The demand for analytical access to dissipative dynamics of non-Markovian character has existed ever since. Simple models can be quick and effective tools in understanding experimental data or assessing dissipative influences on such quantum processes as entanglement and decoherence [14, 15]. However, phenomenological approaches [16–18] are of limited usefulness. What one is really looking for, is a clear relationship with the Hamiltonian at hand. Precisely that prerequisite is met by the Kraus map (10). It provides a fundamental description of both reversible and irreversible behaviour. Mathematical efforts can be kept at a modest level. There is no need to struggle with nasty integral kernels such as the one contained in the Nakajima-Zwanzig equation [19]. For the map (10) all memory effects stem from the fact that the decay time of the pair-correlation function (6) is larger than zero.

ii) In any fundamental theory of quantum dissipation one has to factorise correlation functions in order to escape numerical work. Our factorisation scheme is given by (8). As we saw, this scheme is exact for the examples (11) and (15). One may readily check that (8) also works fine for the interaction $H_1 = \sigma_+ \otimes \sigma_- + \sigma_- \otimes \sigma_+$ between two qubits, at least, if the qubit representing R starts from a pure state. Of course, (8) cannot be true if ρ_R is in a mixed state. On the other hand, it is perfectly possible to handle thermal reservoirs on the basis of the Kraus map (10). For the above-presented example of Jaynes-Cummings dynamics we make the choice $\rho_R = [1 - \exp[-\beta]] \exp[-\beta a^\dagger a]$, where β^{-1} measures the temperature of the reservoir. By (2), the exact density operator $\rho_S(t)$ linearly depends on ρ_R . Consequently, one may perform the expansion $\rho_S(t) = [1 - \exp[-\beta]] \sum_{p=0}^\infty \exp[-\beta p] \rho_{S,p}(t)$, where $\rho_{S,p}(t)$ denotes the density operator of the system corresponding to the initial reservoir state $\rho_R = |p\rangle\langle p|$. This last state is pure, so it makes sense to determine $\rho_{S,p}(t)$ on the basis of the Kraus map (10). As shown by (14), we then end up with an exact description of Jaynes-Cummings dynamics in the presence of a thermal reservoir. If we repeat the foregoing procedure for the Poisson distribution $\rho_R = \exp[-|\alpha|^2] \sum_{p=0}^\infty |\alpha|^{2p} |p\rangle\langle p| / p!$, we even reproduce collapses and revivals of Rabi oscillations. Last, we observe that for some applications it is realistic to choose the reservoir state ρ_R as pure. Examples are interaction between one Rydberg atom and a coherent e.m. field inside a high-quality optical resonator [20], and manipulation of electron spins in semiconductor quantum dots for information processing [21, 22].

iii) Under the van Hove limit the Kraus map (10) becomes $\lim_{\lambda \rightarrow 0} \rho_S(t/\lambda^2) = [\exp[L_1 t] + L_2 \int_0^t ds \exp[L_1 s]] \rho_S$. As anticipated in ii), this result is less general than (5). Hence, the non-Markovian Kraus map (10) is not suited for describing dynamics of purely Markovian type. For the above-discussed example of spontaneous emission there is agreement between (5) and the van Hove limit of (10), owing to the circumstance that the operator $(L_1 + L_2)L_2$ vanishes. To exploit this property in (5), one should invoke the standard integral identity for perturbed

semigroups [23]. In view of the foregoing findings, one might be tempted to exchange (8) for the factorisation scheme underlying (5). This comes down to solving the Nakajima-Zwanzig equation up to second order in λ [24]. Unfortunately, the latter equation relies upon the customary commutator-based expansion of (2). Outside the van Hove limit the use of repeated commutators causes violations of the positivity requirement for the density operator.

iv) In case the composite SR does not start from a factorised state $\rho_S \otimes \rho_R$, the Kraus map (1) is no longer valid. One has to face the fact that the dependence of $\rho_S(t)$ on ρ_S becomes nonlinear [7, 25]. Nevertheless, at a formal level one can still construct exact evolution equations [19]. Furthermore, one can come up with a nonlinear counterpart of (1) [26]. Focusing on the entangled case, *i.e.*, the initial state of SR cannot be written as $\sum_j \rho_{S,j} \otimes \rho_{R,j}$, with $\{\rho_{S,j}\}$ and $\{\rho_{R,j}\}$ density operators, we undertook several attempts to factorise correlation functions and perform a resummation of type (10). We had to conclude that in the presence of entanglement, it is very hard to find a resummation that leaves the positivity of the density operator intact.

v) In constructing a Kraus map for the density operator on the basis of pair-correlation functions, one is not obliged to exclusively perform nearest-neighbour Wick contractions. Let us return to the exact perturbative series for the density operator as generated by (2) and (7). We discuss how one can sum up all terms that contain, apart from nearest-neighbour contractions, precisely one contraction of long-range type. In (7), with n set equal to 5, we perform nearest-neighbour contractions between $U_{\alpha_1}(t_1)$ and $U_{\alpha_2}(t_2)$, as well as between $U_{\alpha_4}(t_4)$ and $U_{\alpha_5}(t_5)$. Upon moving the integral over t_3 to the left, we obtain the form

$$\sum_{\alpha_1 \alpha_2 \alpha_3 \alpha_4 \alpha_5} (-i\lambda)^5 \int_0^t dt_3 \int_{t_3}^t dt_1 \int_{t_3}^{t_1} dt_2 \int_0^{t_3} dt_4 \int_0^{t_4} dt_5 \times \\ \times V_{\alpha_1}(t_1) V_{\alpha_2}(t_2) V_{\alpha_3}(t_3) V_{\alpha_4}(t_4) V_{\alpha_5}(t_5) \otimes U_{\alpha_3}(t_3) c_{\alpha_1 \alpha_2}(t_1, t_2) c_{\alpha_4 \alpha_5}(t_4, t_5). \quad (18)$$

To the left and right of $V_{\alpha_3}(t_3)$ the first-order iterative solutions for $Q(t, t_3)$ and $Q(t_3, 0)$ figure, respectively. Hence, by means of the series $-i\lambda \sum_{\alpha_3} \int_0^t dt_3 Q(t, t_3) V_{\alpha_3}(t_3) Q(t_3, 0) \otimes U_{\alpha_3}(t_3)$, one collects all possible types of long-range contractions. Of course, the foregoing manipulations must be carried out for the adjoint of (7) as well. In doing so, primed times and indices should be used. The desired single long-range contraction is then performed between the potentials $U_{\alpha_3}(t_3)$ and $U_{\alpha'_3}(t'_3)$. Eventually, for the density operator the following contribution is found:

$$\lambda^2 \sum_{\alpha\beta} \int_0^t ds \int_0^t du Q(t, s) V_{\alpha}(s) Q(s, 0) \rho_S Q^{\dagger}(u, 0) V_{\beta}(u) Q^{\dagger}(t, u) c_{\beta\alpha}(u, s). \quad (19)$$

If the double integral on the right-hand side of (10) is replaced by (19), the Kraus map becomes more accurate in the Markovian regime. This can be demonstrated by taking the van Hove limit. One arrives at $\lim_{\lambda \rightarrow 0} \rho_S(t/\lambda^2) = \{\exp[L_1 t] + \int_0^t ds \exp[L_1(t-s)] L_2 \exp[L_1 s]\} \rho_S$. Up to first order in L_2 , this result coincides with (5). Last, we mention that with the help of the above machinery it is straightforward to construct series containing, instead of one, an arbitrary number of long-range contractions. Therefore, we can control the error between the Kraus map (10) and the exact perturbative expansion for the density operator.

vi) If the system is driven by a classical field, the Hamiltonian H_S must be extended with a time-dependent term. Consequently, the operator series $\exp[\pm i \int_0^t dt' H_S(t')]$, which are contained in the time-dependent potentials $\{V_{\alpha}(t)\}$, must be subjected to time-ordering prescriptions. For eqs. (9) and (10) there are no modifications.

vii) The second contribution of the Kraus map (10) is a double integral over time. Let us forget about the integrations and focus on the integrand alone. Clearly, this integrand is

not a density operator, but an entity of the more general form $\sum_m W_m(t)\rho_S W_m^\dagger(t')$. Hence, from (10) one learns that a density operator provides insufficient mathematical freedom for setting up an efficient description of non-Markovian quantum dynamics. With the help of the perturbative expansion (7) one should derive evolution equations for the natural extension of (1) as given above, and make the choice $t = t'$ in due course.

* * *

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